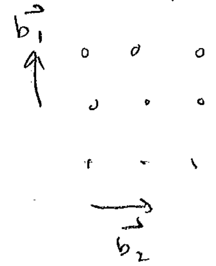
→ Go over "day 4 pg 5" handout

$$\boxed{n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}}$$

Recip. lattice



$$\vec{b}_1 = \left(\frac{2\pi}{a_1}, 0, 0\right)$$

$$\vec{b}_2 = \left(0, \frac{2\pi}{a_2}, 0\right)$$

$$\vec{b}_3 = \left(0, 0, \frac{2\pi}{a_3}\right)$$

"primitive reciprocal lattice vectors"

$$\boxed{\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3}$$

$\vec{G}$ = any general recip. lattice vector

(compare to $\vec{T} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$ general lattice vector from last lecture)

How to calculate $n_{\vec{G}}$?

Before $n_p = \frac{1}{a}\int_0^a n(x)\, e^{-i 2\pi p x/a}\, dx$

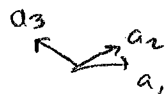
Now $n_{\vec{G}} = \frac{1}{a_1}\frac{1}{a_2}\frac{1}{a_3}\int_0^{a_1}\int_0^{a_2}\int_0^{a_3} n(x,y,z)\, e^{-i2\pi v_1 x/a_1}\, e^{-i2\pi v_2 y/a_2}\, e^{-i2\pi v_3 z/a_3}$

Compact: $$\boxed{n_{\vec{G}} = \frac{1}{\text{vol. of unit cell}}\int_{\text{vol. of unit cell}} n(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, dV}$$

One more time:

The plson reciprocal lattice represent the spatial frequencies we need to include, in order to represent a periodic $n(x,y,z)$ in terms of its Fourier components.

Problem: what if not simple cubic?

Example 

what then?

Then $\vec{b_1}, \vec{b_2}, \vec{b_3}$ not just in $\hat{x}, \hat{y}, \hat{z}$ directions

$\vec{b_1} \perp \vec{a_2}, \vec{a_3}$ → then still have $b_1 \cdot a_2 = 0$, $b_1 \cdot a_3 = 0$ like before

$\vec{b_2} \perp a_1, a_3$

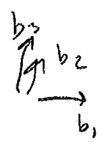
$\vec{b_3} \perp a_1, a_2$

Eqns: with V = vol. of prim. unit cell, $= \vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})$

then

$$\boxed{\begin{aligned} \vec{b_1} &= 2\pi \frac{(\vec{a_2} \times \vec{a_3})}{V} \\ \vec{b_2} &= 2\pi \frac{(\vec{a_3} \times \vec{a_1})}{V} \\ \vec{b_3} &= 2\pi \frac{(\vec{a_1} \times \vec{a_2})}{V} \end{aligned}}$$

gives $\frac{2\pi}{a_1}$ if a_1, a_2, a_3 are all perpendicular

Could come out 

or something

→ Again: these vectors form a lattice of points in "k space", that indicate the Fourier components of (e.g.) $n(\vec{r})$

Cool property: $\boxed{\vec{a_i} \cdot \vec{b_i} = 2\pi \delta_{ij}}$

→ "Kronecker delta" zero unless $i = j$

Awesome theorem

The possible x-ray diffraction peaks are directly connected to the $\vec{G}$ vectors.

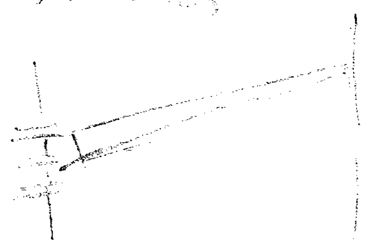
Specifically, $\boxed{\Delta\vec{k} = \vec{G}}$

$\vec{k}_{peak} - \vec{k}_{incident} = \vec{G}$

will give you all diffraction peaks if you try all $\vec{G}$ vectors!

Proof...

first back to 12.3



recall plane wave $\vec{E} = \vec{E}_0 e^{i(\vec{k}\cdot\vec{r} - \omega t + \phi)}$

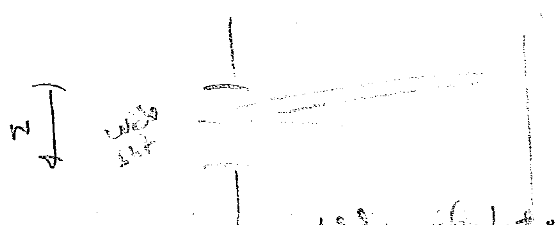
diffraction from 3 slits $E = E_0 e^{i(kr - \omega t + \phi)}$

$E = \sum E_i$

$= E_0 \left(e^{-i\phi} + 1 + e^{+i\phi}\right)$

phase shifts via $e^{i\phi}$

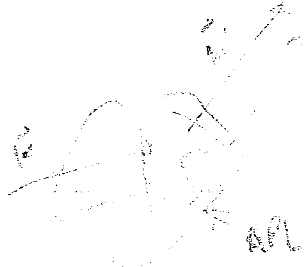
$\phi = 2\pi \left(\frac{\Delta PL}{\lambda}\right)$ $d\sin\theta$



Add up infinite # of phase shifts

$E \propto \int_{-\frac{w}{2}}^{+\frac{w}{2}} e^{i\Delta\phi}\, dy$

back to our case



$$E \propto \int_{\text{volume}} e^{i\Delta\phi}\, dV$$

before $\Delta\phi = 2\pi \frac{\Delta PL}{\lambda}$

$\vec{k}\cdot\vec{r}$ represents how phase of wave changes at a point in space ↔ $\cos(\vec{k}\cdot\vec{r}-\omega t)$

Now $\Delta\phi = \vec{k}\cdot\vec{r} - \vec{k}'\cdot\vec{r}$

$= -\Delta\vec{k}\cdot\vec{r}$ $\Delta\vec{k} = \vec{k}' - \vec{k}$

But... X-rays scatter from electron density, so need to weight by $n(\vec{r})$:

$$F = \int_{\substack{\text{volume}\\ \text{of}\\ \text{crystal}}} n(\vec{r})\, e^{-i\Delta\vec{k}\cdot\vec{r}}\, dV$$

scattering amplitude $E \propto F$

Plug in Fourier representation of $n(\vec{r})$:

$$F = \int_{\substack{\text{vol of}\\ \text{x-tal}}} \left(\sum_{\vec{G}} n_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}\right) e^{-i\Delta\vec{k}\cdot\vec{r}}\, dV$$

$$= \sum_{\vec{G}} \int_{\substack{\text{vol of}\\ \text{x-tal}}} n_{\vec{G}}\, e^{i(\vec{G}-\Delta\vec{k})\cdot\vec{r}}\, dV$$

this $= 0$ unless $\boxed{\Delta\vec{k} = \vec{G}}$! (HW problem Kittel 2.4) (due to oscillations)

That's a large part of the reason why those RLVs are useful

One step further: magnitude of k is not changing, only direction, so $k = k'$

$$\vec{k}' - \vec{k} = \vec{G} \rightarrow \vec{k}' = \vec{G} + \vec{k}$$

$$\vec{k}'\cdot\vec{k}' = (\vec{G}+\vec{k})\cdot(\vec{G}+\vec{k})$$

$$\cancel{k^2} = G^2 + 2\vec{k}\cdot\vec{G} + \cancel{k^2}$$

$$G^2 + 2\vec{k}\cdot\vec{G} = 0$$

if $\vec{G}$ is ~~lattice~~ arbitrary recip. lattice vector then so is $-\vec{G}$, so

$$-2\vec{k}\cdot\vec{G} + G^2 = 0$$

$$\boxed{2\vec{k}\cdot\vec{G} = G^2}$$

Bragg's Law!

(obvious? :))

$$2k\cancel{G}\sin\theta = G^{\cancel{2}}$$

($\cos\phi$ between k + G $= \sin\theta$ from plane)

see picture

recip lattice separated ...

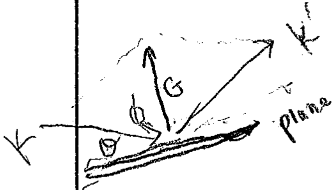
$$2\left(\frac{2\pi}{\lambda}\right)\sin\theta = \frac{2\pi}{d}$$

of planes representing same hkl spacing (HW 2.1)

mag. of G?

$G = \frac{2\pi}{a} \times n$ for ...

or $= \frac{2\pi}{d}$ if you include effect of n as pseudo-planes



hkl = (222)

write as (111) but has $\frac{1}{2}$ the spacing

introduces factor of n

$$2\left(\frac{2\pi}{\lambda}\right)\sin\theta = \left(\frac{2\pi}{d/n}\right)$$

$$2d\sin\theta = n\lambda \checkmark$$

Laue Eqns
Ewald construction } on your own